

		Form Approved OMB NO. 0704-0188	
<p>Public Reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comment regarding this burden estimates or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.</p>			
1. AGENCY USE ONLY (Leave Blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED	
	February 1, 2007	Final (Conf Grant Award) 10/1/05-6/30/07	
4. TITLE AND SUBTITLE		5. FUNDING NUMBERS	
A request to support international conference in frontiers in nanoscale science and engineering.		W911NF-05-1-0562	
6. AUTHOR(S)		8. PERFORMING ORGANIZATION	
Ravindra Pandey		REPORT NUMBER Pandey-Jan2007 (E20633)	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)		10. SPONSORING / MONITORING AGENCY REPORT NUMBER	
Michigan Technological University, Houghton, MI 49931		49297.1-EL-CF	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)		11. SUPPLEMENTARY NOTES	
U. S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211		<p>The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.</p>	
12 a. DISTRIBUTION / AVAILABILITY STATEMENT		12 b. DISTRIBUTION CODE	
Approved for public release; distribution unlimited.			
13. ABSTRACT (Maximum 200 words)			
<p>The international symposium entitled "Frontiers in Nanoscale Science, Technology and Education" was held in Cochin, India from August 16-19, 2006. The main stimulus for organizing this international symposium was various technological interests and goals in the emerging field of nanoscale science and engineering which India shares with the United States. The symposium featured thematically arranged invited and contributed papers. The plenary talk in the symposium was given by Prof. Sumio Iijima, the discoverer of carbon nanotubes, providing a perspective of the field with highlights from his recent work. The topics (e.g. synthesis and processing, theory and modeling, fabrication, energy and environment, materials and devices) were organized along application-oriented themes that deal with specific areas of technology such as nanoelectronics, nano-biotechnology, nano-energetics, and other technology enablers and platforms such as instrument development, materials synthesis and processing and development of modeling as a predictive tool. A major focus of this symposium was on the educational aspect of Nanoscience in which discussions on an array of educational experiences and opportunities designed to provide an integrated and universal curriculum for the academic programs in nanoscale science and engineering.</p>			
14. SUBJECT TERMS		15. NUMBER OF PAGES	
Nanoscale Science and Engineering			
		16. PRICE CODE	
17. SECURITY CLASSIFICATION OR REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION ON THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT UL

NSN 7540-01-280-5500

Standard Form 298 (Rev.2-89)
Prescribed by ANSI Std. Z39-18
298-102

REPORT ON

**The International Symposium on the
Frontiers in Nanoscale Science, Technology and Education
Cochin, India, August 16-19, 2006**

Sponsored by

**Army Research Office, USA
(Contract/Grant - W911NF-05-1-0562)**

Submitted by

Pulickel M. Ajayan, Rensselaer Polytechnic Institute, Troy, NY, USA
(ajayan@rpi.edu)

Shashi Karna, Army Research Laboratory, USA
(skarna@arl.army.mil)

Vikram Kumar, Director, National Physical Laboratory, Delhi, India
(vkmr@mail.nplindia.ernet.in)

Ravindra Pandey, Michigan Tech University, Houghton, MI, USA
(pandey@mtu.edu)

Ashwini K. Srivastava, Mumbai University, India
(aksrivastava@chem.mu.ac.in)

(in collaboration with Harish Bahadur and Harish Chander, NPL, Delhi, India)

Table of Contents

Executive Summary	3
Introduction	6
Symposium Organization	7
Appendix A.	10
Appendix B	13

Executive Summary

The international symposium entitled “Frontiers in Nanoscale Science, Technology and Education” was held in Cochin, India from August 16-19, 2006. The symposium was sponsored by Army Research Office, USA, National Science Foundation, USA, US Air Force Office of Scientific Research, Japan, Department of Science and Technology, India, and Council of Scientific and Industrial Research, India. Additional support was provided by Defense Research and Development Organization, India, Society of Semiconductor Devices, India, National Program on Smart Materials, India and Riber Inc., France.

The main stimulus for organizing this international symposium was various technological interests and goals in the emerging field of nanoscale science and engineering which India shares with the United States. Realizing the significance of this area for upcoming human needs in different disciplines, both countries have come on a common platform. The symposium served as a unique venue, bringing together various participants, to explore collaborative possibilities identifying areas where the complementary strengths of participants will help to create scientific and engineering breakthrough and rapid development to technologies at the nanoscale.

The symposium featured thematically arranged invited and contributed papers. The topics (e.g. synthesis and processing, theory and modeling, fabrication, energy and environment, materials and devices) were organized along application-oriented themes that deal with specific areas of technology such as nanoelectronics, nano-biotechnology, nano-energetics, and other technology enablers and platforms such as instrument development, materials synthesis and processing and development of modeling as a predictive tool. A major focus of this symposium was on the educational aspect of Nanoscience in which discussions on an array of educational experiences and opportunities designed to provide an integrated and universal curriculum for the academic programs in nanoscale science and engineering.

The plenary talk in the symposium was given by Prof. Sumio Iijima, the discoverer of carbon nanotubes, providing a perspective of the field with highlights from his recent work. Overall, the symposium brought together forty invited speakers from United States, India, United Kingdom, Japan, Germany, and Mexico representing academia, industry, and national laboratories. It was attended by about 150 participants, including students, young faculty members, and expert researchers whose work has begun to make impact in nanoscale science and engineering. Representatives from the US National Science Foundation, Department of Defense, Motorola Inc., and other interested and related Indian agencies and industries attended the symposium. All contributory papers were organized in poster to facilitate the dialogue among students and leading scientists of USA, India and several other countries.

A one full-day tutorial on Nanoscience- Fundamentals, theory, materials, and Nano-biotechnology- was organized at the Kochi Institute of Science and Technology. The tutorial session given by the organizers (Ajayan, Pandey, Karna and John) was attended

by over 100 undergraduate, graduate, and postgraduate students selected from all over India and abroad.

The participants in the symposium discussed possible collaborations including exchange and mutual visits, and training of students in each other's institutions under collaborative agreement. Some examples of the potential areas for joint collaborations are: (1) development of new strategies for the synthesis of nanomaterials, particularly soft chemical routes, (2) positioning of these materials (monodispersed & shape defined) in appropriately organized arrays using lithographic techniques or templating methods (molecular or supramolecular assembly) or deposition inside the void spaces of nanoporous host materials, (3) development of nanodevices based on photo, electro, magneto, thermo or chemo-active properties, (4) applications and integration of nanodevices based on quantum phenomena, nonlinear optics, photonics, catalysis, and solar cells, (5) nanoscale energy sources, (6) modeling and simulation algorithms and tools, and (7) development and implementation of the academic program with interdisciplinary training and interactions for undergraduate and graduate students in nanoscale science and engineering.

The main observations and recommendations based on the presentations at the conference are the following:

- **Theory and modeling tools development**

- Integration of theoretical methods based on *first-principles* Quantum Mechanics, Force field-based Molecular Mechanics, Molecular dynamics, and Mesoscale simulation methods for computation of the structure property evolutions in nanoscale materials and structures.
- *First principles*-based theoretical and modeling tools to reliably predict structure and response properties of nanoscale materials, such nanotubes, quantum dots, and self-assembled monolayer systems.
- Physically-based computational tools to simulate nano-scale devices. For example, a SPICE-type modeling tool including transport and materials parameters of nano-scale materials.

- **Materials growth and synthesis**

- Need for the development of the experimental techniques for scaled-up production of carbon and other nanotubes in sufficient purity.
- Need for the development of experimental techniques to assemble nanotubes into useful configurations for novel technological applications.
- Development of functional nanomaterials for applications in energy conversion, energy storage and energy efficiency.

- **Device fabrication and testing**
 - Opportunities in the fabrication of large and complex systems with nanowires integrating III-V materials on Si wafer for ultra-fast nano-electronic and photonic devices. Integration of nanodevices with the Si-technology was identified a major requirement for rapid commercialization of the technology.
 - Development of a nanosensing platform that utilizes quantum dots, proteins, and single electron transistors (SETs) to form a chemical or biological detection system.
- **Nano-bio science and technology**
 - Fundamental understanding of the interaction between nano-scale and biological materials. Response and functional properties of nano-bio materials
- **Education**
 - Integration of the Nanoscience and engineering in undergraduate curricula that provides detailed understanding of the foundational aspects, namely the underlying science, instrumentation, metrology, and technological applications and engineering techniques associated with the nanotechnology.
- **Environmental and Societal impact**
 - Research directed at understanding environmental and health impacts of nanomaterials.
 - Focused effort on educating the society in general on the science and engineering aspects of nanotechnology.

Additionally, a number of specific issues and a need for open exchange of ideas, publication in research results in journals easily accessible to students in developed as developing nations were identified. An exchange program between the academic institutions in India and their counterparts along with leading industrial research organizations was also identified as catalysts for rapid progress in nanotechnology. Finally, increased funding by various government agencies and industries with focused investment on Nanoscience education and research efforts was identified as the most critical need.

With US as the Leader in Technology and India being a front runner among the developing nations, the symposium was extremely successful and mutually beneficial to the scientific communities from both countries along with scientists from other countries such as Japan, Germany, and United Kingdom.

Introduction

Nanoscale science and technology have emerged over the past decade as the forefront of science and technologies. The intersecting fields of study that create this domain of science and engineering perfectly typify the rapid, multidisciplinary advancement of contemporary science and technology. New experimental techniques, such as scanning probe microscopy, nano-lithography, and powerful computer simulations combined with the emergence of new form of materials such as the carbon nanotubes, nanowires, and precisely controlled quantum dots, have opened new worlds to physical, chemical, mechanical, material, and biological scientists and engineers, whose understandings of nature, in turn, have allowed further development of experimental tools and techniques that continue to unravel the mysteries of the physical world at the nanoscale. These developments have led individual scientists in respective institutions and countries to advance the subjects of their expertise at an unprecedented speed. However, there has been generally a lack of a converging goal from the systems applications and technological development points of view. A technology involving nano-scale science and engineering by its very nature requires combined effort of experts trained in varied areas of disciplines. Moreover, since this newly emerging area requires new paradigms not only in systems developments and integration, but also in fabrication, manufacturing, commercialization, and marketing, a forum providing multi-national platform addressing all the associated issues is expected to expedite the technology developments at nano-scale. The purpose of this "International symposium on the Frontiers of Science, Engineering and Education at Nanoscale" was to provide such an international venue for a focused and productive dialogue among scientists, engineers and technologists.

The United States of America has been a technological leader in the past century in such vast areas as the microelectronics, medical diagnostics, health care, and most recently, fighting terrorism. The USA has also been a leader in research and developments in the areas of nano-scale materials, engineering, characterization tools, modeling and application-oriented engineering developments. The recent emphasis on nanoscale science, engineering and education through the National Nanotechnology Initiatives (NNI) has further intensified and solidified the fundamental and applied research and developments across many disciplines, particularly in nanoscale materials, nanoelectronics and nanophotonics in the USA. Yet, as the demand for new concepts and well-trained experts in the emerging areas of nanoscale science and technology continues, the USA will greatly benefit from the vast accumulation of technical know-how and well-trained resources in other countries, especially India.

India has emerged as a "front runner" among developing nations researching into nanoscale sciences and engineering, and is now taking steps to build an economically and technologically sustainable nanotech sector. India's president A.P.J. Abdul Kalam, has long championed the growing field as a means to bolster the country's economy.

"[Nanotechnology] is the field of the future that will replace microelectronics and many fields with tremendous application potential in the areas of medicine, electronics

and material science.” said Kalam in a recent speech, while stating elsewhere that nanotech will be a major driver to “*transform India into a developed nation by 2020.*”

India has taken a step ahead of many countries in placing specialized curricula for undergraduate and graduate students in a multidisciplinary nanoscale science and has begun to produce highly trained technical talents in this new area. India has already begun to make impact in such areas as the nanoscale materials and engineering applications in fighting terrorism, particularly involving chemical and biological agents, medical and health care, and space technology applications. Furthermore, with its growing emphasis on encouraging small innovative industries to participate in the new technological revolution, highly efficient mechanism for transitioning technology from the R&D level to commercial and military products, and open policies for international investment, India is but poised to take a leading role in the nanotechnology driven economic development.

The international symposium on “Frontiers of Science, Engineering and Education at Nanoscale” provided a platform for a wide range of discussions between participants from several countries regarding technological challenges, system integration and commercialization. The symposium has developed not only bilateral opportunities between US and India, but has also provided a forum for potential interaction with other countries. Specifically, it was focused on initiating collaborations among academia, and government laboratories, and industry partners about a rapid development of nanotechnology that is going to enable advances in several research areas, such as electronics, sensors, biotechnology. Efforts were devoted to create more interest in the stream through poster sessions for research students and young faculty members.

Symposium Organization

The symposium featured thematically arranged invited and contributed papers (poster sessions). The topics were organized along application-oriented themes that deal with specific areas of technology such as nanoelectronics, nano-biotechnology, chemical and biological sensors, nano-energetics, and other technology enablers and platforms such as instrument development, materials synthesis and processing and development of modeling as a predictive tool. The symposium also included discussions on an array of educational experiences and opportunities designed to provide an integrated introduction to three crucial aspects of nanoscale work: the underlying science, possible scientific and engineering applications, and the societal implications of this still unfolding realm of science and engineering. All technical sessions were chaired by an eminent researcher in the area.

The details of the schedule of the symposium are given in Appendix A.

The abstracts for the invited talks for the oral session and contributed talks for the poster sessions are given in Appendix B and C, respectively.

The participants discussed possible collaborations including exchange and mutual visits, and training of students in each other's institutions under collaborative agreement. Some examples of the potential areas for joint collaborations are: (1) development of new strategies for the synthesis of nanomaterials, particularly soft chemical routes, (2) positioning of these materials (monodispersed & shape defined) in appropriately organized arrays using lithographic techniques or templating methods (molecular or supramolecular assembly) or deposition inside the void spaces of nanoporous host materials, (3) development of nanodevices based on photo, electro, magneto, thermo or chemo-active properties, (4) applications and integration of nanodevices based on quantum phenomena, nonlinear optics, photonics, catalysis, and solar cells, (5) nanoscale energy sources, (6) modeling and simulation algorithms and tools, and (7) development and implementation of the academic program with interdisciplinary training and interactions for undergraduate and graduate students in nanoscale science and engineering.

The main observations and recommendations based on the presentations at the conference are the following:

- **Theory and modeling tools development**
 - Integration of theoretical methods based on *first-principles* Quantum Mechanics, Force field-based Molecular Mechanics, Molecular dynamics, and Mesoscale simulation methods for computation of the structure property evolutions in nanoscale materials and structures.
 - *First principles*-based theoretical and modeling tools to reliably predict structure and response properties of nanoscale materials, such nanotubes, quantum dots, and self-assembled monolayer systems.
 - Physically-based computational tools to simulate nano-scale devices. For example, a SPICE-type modeling tool including transport and materials parameters of nano-scale materials.
- **Materials growth and synthesis**
 - Need for the development of the experimental techniques for scaled-up production of carbon and other nanotubes in sufficient purity.
 - Need for the development of experimental techniques to assemble nanotubes into useful configurations for novel technological applications.
 - Development of functional nanomaterials for applications in energy conversion, energy storage and energy efficiency.
- **Device fabrication and testing**
 - Opportunities in the fabrication of large and complex systems with nanowires integrating III-V materials on Si wafer for ultra-fast nano-electronic and photonic devices. Integration of nanodevices with the Si-technology was identified a major requirement for rapid commercialization of the technology.

- Development of a nanosensing platform that utilizes quantum dots, proteins, and single electron transistors (SETs) to form a chemical or biological detection system.
- **Nano-bio science and technology**
 - Fundamental understanding of the interaction between nano-scale and biological materials. Response and functional properties of nano-bio materials
- **Education**
 - Integration of the Nanoscience and engineering in undergraduate curricula that provides detailed understanding of the foundational aspects, namely the underlying science, instrumentation, metrology, and technological applications and engineering techniques associated with the nanotechnology.
- **Environmental and Societal impact**
 - Research directed at understanding environmental and health impacts of nanomaterials.
 - Focused effort on educating the society in general on the science and engineering aspects of nanotechnology.

The symposium was extremely successful and mutually beneficial to the scientific communities from USA and India along with scientists from other countries. It also provided an opportunity to make an important contribution to upgrading the research skills of well-prepared young scientists, together with establishing working relationships for future research and development in the area of nanoscale science and engineering.

Acknowledgements

The support of Dwight Woolard at ARO and Dr. Rajinder Khosla at NSF was critical to the success of the symposium. A special word of appreciation to Poornima Ajayan, Harish Bahadur, Harish Chander, Anatharaman, and Y. Raman for their help in the organizational aspects of the symposium. Finally, financial support from National Science Foundation, USA, Army Research Office, USA, US Air Force Office of Scientific Research, Japan, Department of Science and Technology, India, and Council of Scientific and Industrial Research, India, Defense Research and Development Organization, India, Society of Semiconductor Devices, India, National Program on Smart Materials, India, Riber Inc., France and Michigan Technological University, USA is acknowledged.

Appendix A : Schedule

Aug 15, 06 (Tuesday)

3-5 PM Registration *Cochin Institute of Technology*
3-5 PM Registration *Taj Malabar*

Aug. 15, 2006 (Tue) Cochon Institute of Technology

Tutorial - 1.00 PM- 5.00 PM Students/Participants

*P. Ajayan, RPI Synthesis
R. Pandey, MTU Theory
S. Karna, ARL Devices (Electronics and Photonics)
George John Chemistry, Nanomaterials and Biomimetics*

Aug 15, 06 (Tue) Taj Malabar
Registration 7.00-10.00 PM

Aug 16, 06 (Wed) Taj Malabar
Registration 7-10 AM

Synthesis and Processing (Chair-Karna, ARL)

Morning

A-1	8.30	<i>Inauguration/Welcome</i>	
	9.00	<i>Sumio Iijima, Japan</i>	<i>Carbon Nanotubes: production, characterization and applications</i>
A-2	9.30	<i>Narayan Das, NMRL Cochin</i>	<i>Nanotechnology - A Route to Functional Materials</i>
A-3	10.00	<i>Pulickel Ajayan, RPI</i>	<i>Engineering Carbon Nanotube Architectures</i>
A-4	10.30	<i>Archita Patnaik, IIT Madras</i>	<i>Structure and Dynamics in a Self-Organized C60–Fullerene Dyad</i>

11.00 Coffee Break

(Chair- Varshney, NSF)

A-5	11.15	<i>Robert Geer, SUNY Albany</i>	<i>Bioinspired Materials for Nanoelectronics</i>
A-6	11.45	<i>O. N. Srivastava, BHU, Varanasi</i>	<i>Studies of Synthesis, Growth, Characterization of Some Nanomaterials</i>
A-7	12.15	<i>A. K. Tyagi, BARC</i>	<i>Nano-Ceramics by Chemical Routes</i>
A-8	12.45	<i>M. Anatharaman, Cochin</i>	<i>Towards Transparent Magnetic Materials—By Excitonic Confinement</i>
A-9	1.15	<i>Harish Bahadur, NPL</i>	<i>Structure Property Correlation of Nano-Structured Thin Films of ZnO</i>

1.30 Lunch

Afternoon Education (Chair-Ajayan, RPI)

A-10	2.30	<i>Usha Varshney, NSF</i>	<i>National Science Foundation Support for Research and Education in Nanoscale Science, Engineering and Technology</i>
A-11	3.00	<i>S. Ranganathan, IISc</i>	<i>Evolution of Materials Education - The Indian Scenario</i>

A-12	3.30	<i>John Jaszcak, Michigan Tech</i>	<i>Introducing Nanotechnology Education in the Undergraduate Curriculum</i>
A-13	4.00	<i>Robert Vajtai, RPI</i>	<i>Life in the nano world: the Molecularium project</i>
A-14	5.00	<i>Pradeep Haldar, SUNY Albany</i>	<i>Educating the Workforce for the New Nanotechnology Industry</i>

5.30 *Tea Break and Poster Session I*
 7.00 *Cultural Program*
 8.30 *Dinner*

Aug 17, 2006 (Thursday)

Theory and Modeling (Chair-Pandey, Michigan Tech)

<i>B-1 Systems</i>	8.00	<i>Shashi Karna, ARL</i>	<i>Electron Transport in Molecular and Nano-scale</i>
<i>B-2</i>	8.30	<i>Brett Dunlap, NRL</i>	<i>Precisely Variational Quantum Chemistry via Analytical Density Functional Theory</i>
<i>B-3</i>	9.00	<i>Dilip Kanhere, Univ of Pune</i>	<i>Thermodynamics of Clusters : Size Sensitive Heat Capacities and Higher than Bulk Melting Point</i>
<i>B-4</i>	9.30	<i>Swapan Pati, JNCASR, Bangalore</i>	<i>Stability of Nanoclusters and NDR Phenomena in Molecular Systems</i>
<i>B-5</i>	10.00	<i>Vinod Tewary, NIST</i>	<i>Theory of Mössbauer Spectrum of a Single-Walled Carbon Nanotube</i>

10.30 *Coffee Break*
(Chair- Narayan Das, NMRL, Cochin)

<i>B-7</i>	11.15	<i>Amitesh Maiti, LLNL</i>	<i>Multiscale Modeling with Carbon Nanotubes</i>
<i>B-8</i>	11.45	<i>Masayoshi Nakano, Osaka</i>	<i>Theoretical Study of Exciton Dynamics of Dendritic Systems</i>

Characterization

<i>B-9</i>	12.15	<i>S. Pennycook, Oak Ridge</i>	<i>Characterization of Nanostructures with Single Atom Sensitivity through Aberration-Corrected STEM</i>
<i>B-10</i>	12.45	<i>K. Muraleedharan, DMRL, Hyderabad</i>	<i>Characterization of MW-CNTs synthesized by thermal and PE CVD for Display Devices</i>
<i>B-11</i>	1.15	<i>Ghatu Subhash, Michigan Tech</i>	<i>Characterization of Nanoporous Diatom Frustules using Nanoindentation</i>

1.30 *Lunch*

Fabrication, Energy and Environment *(Chair-Kumar, NPL)*

<i>B-13</i>	3.30	<i>Laura Lewis, Brookheaven</i>	<i>Nanoscience and the Energy Challenge: The U. S. Department of Energy's Nanoscale Science Research Centers</i>
<i>B-14</i>	4.00	<i>S. Ramaprabhu, IIT Madras</i>	<i>Energy-Related Applications of Carbon</i>
<i>B-15</i>	4.30	<i>Vijay Mohan, NCL Pune</i>	<i>Applications of Hybrid nanomaterials for Electrochemical Energy Storage</i>

<i>B-16</i>	<i>5.00</i>	<i>Mauricio Terrones, IPICYT, Mexico</i>	<i>Novel Effect of Electron Irradiation in Nanostructures</i>
	<i>5.30</i>	<i>Tea Break and Poster Session II</i>	
	<i>8.00</i>	<i>Banquet</i>	
			<i>Aug 18, 06 (Friday)</i>
		<i>Materials and Devices</i>	<i>(Chair-Srivastava, Mumbai)</i>
<i>C-1</i>	<i>8.30</i>	<i>Vikram Kumar, NPL</i>	<i>Overview of Nanotechnology Research in India</i>
<i>C-2</i>	<i>9.00</i>	<i>Bhasker Rao K, DMSRDE Kanpur</i>	<i>Synthesis and study of characteristics of Nanomaterials for different applications</i>
<i>C-3</i>	<i>9.30</i>	<i>Yoshio Bando, NIMS, Japan</i>	<i>Inorganic Nanotubes</i>
<i>C-4</i>	<i>10.00</i>	<i>Murali Sastri, Tata Chemicals</i>	<i>Shape matters in nanomaterials</i>
	<i>10.30</i>	<i>Coffee Break</i>	
			<i>(Chair-Harish Bahadur, NPL)</i>
<i>C-5</i>	<i>10.45</i>	<i>Horst Hahn, Germany</i>	<i>Novel Aspects of Property Control in Nanostructured Materials</i>
<i>C-6</i>	<i>11.15</i>	<i>A. K. Srivastava, Univ of Mumbai</i>	<i>Carbon Nanotubes as Electrochemical (Bio)Sensors</i>
<i>C-7</i>	<i>11.45</i>	<i>Saif Islam, UC Davis</i>	<i>Integrating and Accurate Positioning of 1D Nanowires in Devices and Circuits</i>
<i>C-8</i>	<i>12.15</i>	<i>Asim Ray, Univ of London</i>	<i>Electronics with Dyes</i>
	<i>1.15</i>	<i>Lunch</i>	
		<i>Nano-Bio</i>	<i>(Chair-Anatharaman, CUST)</i>
<i>C-10</i>	<i>2.00</i>	<i>Craig Friedrich, Michigan Tech</i>	<i>Protein Nanosensors for Multi-Scale Technologies</i>
<i>C-11</i>	<i>2.30</i>	<i>Koel Chaudhary, IIT Kharagpur</i>	<i>Imaging Spermatozoa using Atomic Force Microscopy -</i>
<i>C-12</i>	<i>3.00</i>	<i>Saber Hussain, AFRL</i>	<i>Implication of nanotechnology and future health effects: Biological and Environmental Effect of Nanomaterials</i>
<i>C-13</i>	<i>3.30</i>	<i>C. P. Joshi, Michigan Tech</i>	<i>Applications of Nanoscale Sciences to Cell Wall Biotechnology in Trees</i>
<i>C-14</i>	<i>4.00</i>	<i>George John, CUNY</i>	<i>Biobased Organic Synthesis: Novel Building Blocks for Soft Nano Materials by Bottom-Up Design</i>
<i>C-15</i>	<i>4.30</i>	<i>Satya Prakash, McGill Univ</i>	<i>Designing micro, macro, and nano artificial cells: potentials and limitations</i>

Concluding Remarks

Appendix B : Abstracts of Invited Talks

A-1

Carbon Nanotubes: production, characterization and applications

Sumio Iijima
Research Center for Advanced Carbon Materials (AIST),
Meijo University and NEC

Many unique properties of CNTs depend on their structures and morphologies. When come to detailed comparisons between experiment and theory, well-controlled and characterized specimens (diameter, length, quantity, chirality, structural perfection, impurity, homogeneity) will be eventually needed. This is also true for their industrial applications to match their requirements. Recently two very important breakthroughs in single-wall carbon nanotube (SWCNT) growth were made in our laboratories at AIST (1). One is a floating catalyst-assisted CVD method of growing SWCNTs. The method can provide controlled tube diameters and extremely high purity tubes with high production yield according to optical spectroscopic characterization. The other is the “Super-Growth” of CNTs, which can grow vertically on various substrates including metal foils as high as several one centimeters. A precise control of small amount of water during the CVD reaction is a crucial point for such efficient growth. On the basis of the superior properties of the super-growth SWCNTs we started to develop a super-capacitor, which can be used for high power density energy storage. Lastly, the importance of characterization of nano-structured materials will be demonstrated by showing the latest results of atomic structures of CNTs and their modifications, which have been revealed by an ultra-high resolution TEM with a spherical aberration corrector. Individual carbon atoms, local atomic defects of SWCNTs and individual fullerene molecules were directly recorded. Dynamic behaviors of those atoms and defects as well as doped metal atoms inside the tubes are of interest in terms of more sophisticated device application of CNTs (2).

(1) T. Saito, et al., J. Phys. Chem. B, **109**, 10647-10652 (2005). D. Futaba et al., Science **306**, 1362-1364 (2004).
D. Futaba et al., Phys. Rev. Lett. **95**, 056104 (1)-(4) (2005).
(2) A. Hashimoto, et al., Nature, **430**, 870-873 (2004). K. Urita, et al., Phys. Rev. Lett, **94**, 155502(2005).
Z. Liu, et al., Phys. Rev. Lett., **95**, 187406(1)-(4) (2005).

Email : ijimas@ccmfs.meijo-u.ac.jp

A-2

Nanotechnology - A Route to Functional Materials
Narayan Das
NMRL
Cochin, India

A-3**Engineering Carbon Nanotube Architectures**

Pulickel Ajayan

Department of Materials Science

Rensselaer Polytechnic Institute, Troy, New York 12180 United States

Carbon nanotubes are fascinating materials from the point of view of structure, form, growth and properties. The biggest challenge however is to assemble nanotubes into various architectures useful for specific applications. The talk will focus on the recent developments in our laboratory on the fabrication of carbon nanotube based architectures tailored for various applications. Various organized architectures of multiwalled and singlewalled carbon nanotubes can be fabricated using relatively simple vapor deposition techniques. The work in attaining control on the directed assembly of nanotubes on various platforms will be highlighted. Our efforts on the strategies of growth and manipulation of nanotube-based structures and in controllably fabricating hierarchically branched nanotube and nanotube-hybrid structures will be discussed. We have pursued several novel applications for these structures, for example, as nanostructured electrodes for sensors, electrical interconnects, unique filters for separation technologies, thermal management systems, multifunctional brushes, and polymer infiltrated thin film and bulk composites. A perspective of the field based on the work done by the author over a period of more than decade will be presented here with highlights from recent work and thoughts on future implications of the field.

A-4**Structure and Dynamics in a Self-Organized C₆₀–Fullerene Dyad**

Archita Patnaik

Department of Chemistry

Indian Institute of Technology Madras

Chennai, Tamilnadu 600 036 India

Understanding the intermolecular interactions in carbon nanomaterials is an important step toward rational designing of functional nanoscopic architectures. Precise control of the geometry of the self-assembled structure allows fine-tuning of the functional properties of these materials in building nanoelectronics. A careful premeditated design of Fullerene[60] based donor–bridge–acceptor dyad systems aids in controlling their electronic properties and self–assembly for application in molecular electronics. The talk will focus on one such dyad system and its structure–property correlations leading to molecular rectification.

A novel methano fullerene dyad based on a hydrophobic – hydrophilic- hydrophobic network has been designed and synthesized. The ab initio geometry optimized structure with B3LYP / 3-21G* level of theory indicated a ground state intramolecular charge-transfer complex formation between the donor and the acceptor moieties of the dyad, further corroborated by the large magnitude of the calculated dipole moment, natural population analysis and the spatial electron density distribution of the dyad's HOMO. Concentration and solvent polarity controlled structure architectures from the self-assembly of the - electronic amphiphile resulted in spherical fractal aggregates of ~10 nm when extracted from THF into water. Molecular dynamics simulations revealed the unit cluster to such a form involves an aggregation number ~90 with predominant soft associative molecular interactions, corroborating the octadecahedral model proposed for the cluster growth. A rectifying junction operating at an applied bias voltage of ± 3 V with an optimum rectification ratio of 158 at 3 V has been obtained from the LB monolayer film of the dyad with a verification of molecular rectification obtained from the symmetrical I-V curves from the centrosymmetric bilayers of the dyad.

A-5

Bioinspired Materials for Nanoelectronics

Robert Geer
College of Nanoscale Science & Engineering
University at Albany-SUNY
Albany, NY 12203 United States

The need for nanoscale structures in next generation electronic devices has directed attention toward the use of novel motifs for the construction of the essential interconnect networks. The formation of such nanowire assemblages directly confronts several challenges including scalability, self assembly and nanoscale patterning. Along with others, we have recognized that biomaterials may provide a potential solution. While biomaterials generally do not possess sufficient conductivity they may serve as templates for assemblage of conducting moieties such as aromatic rings or metallic components. Polypeptides are especially attractive templates as they fold by established rubrics, undergo intermolecular self-assembly, present a wide variety of functionality and are chemically robust. Of particular interest, β -sheet forming sequences have been long recognized to form well-ordered aggregates, and under some conditions form fibrillar structures, the best known representatives of which are amyloid fibrils. Adapting the pioneering work of Tirrell, a *de novo* genetically engineered family of polypeptide sequences has been prepared that self assembles to form nanofibrils that can be oriented via surface-directed assembly. These fibrillar structures have been adapted to 2-point electronic test circuits for electrical investigation. In addition, parallel efforts have investigated direct metallization of these fibrillar structures for the formation of hybrid nanowires to exploit the biological beta-sheet self-assembly.

A-6

Studies of Synthesis, Growth, Characterization of Some Nanomaterials

O. N. Srivastava
Department of Physics,
Banaras Hindu University, Varanasi-221005

The talk will focus on the growth, synthesis, characterization and applications of some nanomaterials. The case of organized structures of (a) Carbon nanotubes (b) ZnO nanorods and their properties/applications will be highlighted. In addition to nanophases /structures of TiO₂, Cu₂O, SnO₂ SiC will also dealt with. The application of organized CNT structures in hydrogen production at the expense of only half as much energy has required conventionally (corresponding to 1 volt) will be described and discussed. In regard to ZnO possibly the highest number of nanovariants e.g. nanowires, nanoneedles, nanopods, nanorings, nanocomb, nanonail and several others have been reported. However, it has not yet been quite possible to synthesized organized nanostructures of ZnO. The formation of organized ZnO nanorods together with their photoluminescence properties with indication of blue in addition to usual green emission will be described and discussed. This presentation will also cover the formation of nanostructures of Cu₂O, SnO₂ and SiC. The synthesis and advantages of preparation of certain medicines e.g. amphotericin B in nanoform is of significant advantage to reduce the toxic effects of the medicine. This work which Physics and Medicine Dept. of B.H.U. are jointly carrying out will also be outlined and discussed.

A-7

Nano-Ceramics by Chemical Routes

A. K. Tyagi
Chemistry Division,
Bhabha Atomic Research Centre
Mumbai - 400 085 India

The nano-ceramics are potential candidates for a variety of technological applications and hence their commercial value is increasing tremendously. Depending up on the final application, oxide ceramics are used in the form of sintered body having the desired shape, size and microstructure. Hence, the synthesis of powder with controlled and required characteristics is of the utmost importance. The shape, size, extent of agglomeration and purity are the important characteristics for deciding the powder quality. There are a number of methods for preparing the nanocrystalline materials viz., inert gas condensation, physical vapor deposition, laser ablation, chemical vapor deposition, sputtering etc. In addition, there are a number of chemical routes also. Among the available chemical routes, the combustion technique is capable of producing the nanocrystalline powders of the oxide ceramics at lower calcination temperature in a surprisingly short time, without any elaborate laboratory facilities. This process involves a combustion reaction between a fuel (e.g. glycine, citric acid, urea etc.) and an oxidizer (i.e., metal nitrates). Depending on the system, the selection of a suitable fuel is a crucial step to begin with. In our group a wide ranging functional materials, viz. nuclear materials, ionic conductors, catalysts and optical materials, have been prepared by combustion route. The specific examples are ceria, thoria, barium polytitanates, barium and strontium thorate, doped ceria, SrCeO_3 , Sr_2CeO_4 , $\text{Zr}_{0.8}\text{Ce}_{0.2}\text{O}_2$, YSZ, $\text{La}_{1-x}\text{Ca}_x\text{CrO}_3$, rare-earth ortho-ferrite. A number of techniques like XRD, HT-XRD, surface area analyzer, SEM, TEM, sinterability, Raman spectroscopy, dynamic light scattering, small angle x-ray/neutron scattering, dilatometer etc. were used for detailed characterization. It was shown to be a simple and cost effective technique, which results in the phase pure, nanocrystalline powders having high surface area and better sinterability. The crucial role of process parameters, especially fuel-to-oxidant ratio, on powder characteristics will be discussed in detail. This method could be extended to prepare thermodynamically metastable phases also, which are difficult to prepare by a conventional ceramic method. The effect of heating rates was found to have a strong bearing on sinterability of the nano-powders while retaining the sub-micron grain size. The versatility and capability of the combustion technique as a preparative method for a variety of nanocrystalline powders of oxide ceramics will be discussed in this talk. A few typical examples of their optical and electrical properties will also be elaborated.

A-8

Towards Transparent Magnetic Materials—By Excitonic Confinement

M. R. Anantharaman
Cochin University of Science and Technology
Cochin, Kerala 682022 India

The prospect of finding transparent magnetic materials are very bright with the advent of nanoscience and nanotechnology. Nature does not produce magnetic materials and it has to be made by man. Transparent magnetic materials find innumerable applications in xerox technology, magneto-optical recording, magnetic field controlled optical modulators, magneto-optical displays and switching devices.

It is known that particles in the nanoregime exhibit superlative physical, magnetic, optical, chemical and electric properties with respect to their coarser sized cousins. In magnetic materials, finite size effects are manifested in the form of quantum magnetic tunneling, superparamagnetism, single domain nature and shift in optical absorption edges. Their large surface to volume ratio provides excellent scope for the modification of their properties due to the large reduction in their linear dimension and high lattice strain. Optical properties of magnetic materials change enormously including the bandgap due to small wave function overlapping. In order to study the excitonic confinement, ultrafine maghaemite particles are

incorporated inside polystyrene matrix by the strong ion exchange process. It has been found that, in the weak field excitonic confinement, a maximum of 0.64 eV can be blue shifted and if the particle size can be further reduced to the ‘dot’ level, a maximum shift of 1.6 eV can be achieved. This augurs well for producing optically transparent magnetic materials. The alloying induced blueshift in magnetite based ferrofluids will also be dealt with. The details of the synthesis of magnetic nanocomposites and the blue shift by excitonic confinement are discussed in this paper.

A-9

Structure Property Correlation of Nano-Structured Thin Films of ZnO

Harish Bahadur

National Physical Laboratory

New Delhi, Delhi 110012 India

Nanostructured zinc oxide is of current technological importance in a variety of sensors and molecular electronics applications. Due to high mechanical stability, nanowires of ZnO are a promising candidate as probe for AFM cantilever. However, a sharp needle shaped structure would still be a better option for the tip of the AFM probe. The nanostructures exhibit novel electrical, mechanical, chemical and optical properties which are believed to be due to the surface confinement effects of nanostructures in one dimension (1 D). These 1 D objects are of great importance in understanding some basic physics related phenomena in the low dimension systems to form the basis of next generation high performance nanodevices.

This presentation focuses on our investigations on the structure property co-relationship of thin films of ZnO grown by sol-gel spin process and RF sputtering method. A comparison between the physical characterization and the nanostructures of the two types of films has been presented and the results are discussed in terms of the fundamental considerations governing the growth kinetics of the ZnO films. X-ray diffraction investigations have revealed the crystalline nature of the films and the photoluminescence studies of all these films have shown quantum confinement. The sol-gel films were grown by using zinc nitrate and zinc acetate as the precursor materials on an oxidized Si substrate. The films prepared using zinc nitrate have shown a polycrystalline structure having two different morphologies. SEM micrographs delineated a dense networking of needle-shaped and island-shaped morphologies. At higher magnification, in general, the fine scale sharp needles converged to a tip is of the order of 15-20 nm, whereas the almost spherical shaped island appeared in two diameters of the range 5 to 10 nm and 0.5 to 1mm. Importantly, the needles and island morphologies exhibited the homogeneous and uniform distribution over the entire film. On the other hand, films grown by zinc acetate as the precursor have shown much smoother needle shaped morphologies embedded in the film microstructure as observed by SEM. Further characterization under the TEM exhibited that the film with uniform microstructure consisted of distribution of nanosized grains of the order of 5 nm. It is important to mention here that nano-grained microstructure grown by two different precursors is almost similar. However, the morphologies developed in these films were more prominent in the case of zinc nitrate precursor (needles and island) as compared to the zinc acetate precursor where very fine needles were observed. Selected area electron diffraction patterns in the case of both the precursors as starting material has shown the presence of different rings corresponding to different planes of hexagonal ZnO crystal structure. The RF sputtered films have shown the formation of nanorods of ZnO.

A-10**National Science Foundation Support for Research and Education
in Nanoscale Science, Engineering and Technology**

Usha Varshney
Electrical and Communications Systems
National Science Foundation
Arlington, VA 22230

The emergence of nanoscale science, engineering, technology and education has led to revolutionary advances as drivers of the global economy. An increase in U.S. spending for nanotechnology over the past five years reflects the Administration's continuing support for expanding knowledge, strengthening the US economy, supporting national security and enhancing the quality of life for all citizens. The U.S. National Nanotechnology Initiative (NNI) is a long-term research and development program announced in January 2000 that coordinates 25 federal agencies and departments having a total budget of about \$ 1.2 billion in fiscal year 2006, of which the estimated budget for the National Science Foundation (NSF) is \$344 million. The NSF supports collaborative research and education in nanoscale science and engineering through single investigator research, interdisciplinary research and education teams, nanotechnology science and engineering centers, exploratory research, networks and user facilities. NSF also supports nanotechnology research and education through focused initiatives and core programs. These various support mechanisms will be presented. NSF's goal is to support fundamental research to catalyze synergistic science and engineering research and education in emerging areas of nanoscale science and technology. In the past five years nanotechnology has experienced considerable progress in expanding from passive nanostructured components to active nanosystems, and from scientific discovery to technological innovation. Challenges facing the nanotechnology community and its sponsoring agencies will be addressed.

A-11**Evolution of Materials Education - The Indian Scenario**

Srinivasa Ranganathan
Indian Institute of Science
Bangalore, Karnataka 560012 India

1923 marks the beginning of formal education in a materials related field, when the farsighted vision of Pandit Madan Mohan Malaviya led to the establishment of the first Department of Metallurgy in India at the Banaras Hindu University. In 1964 a school in Materials Science was organized in the Indian Institute of Technology, Kanpur and marked the broadening of materials programme in India. The advent of nanoscience in the late nineties has led to some tentative efforts at education in this field. We will survey these developments in India over the past eight decades and compare them with global developments. The slice of materials education will also be put in the context of higher technical education in India.

A-12

Introducing Nanotechnology Education in the Undergraduate Curriculum

John Jaszczak
Physics Department
Michigan Technological University
Houghton, Michigan 49931-1295 United States

A team of faculty at Michigan Technological University (MTU) has developed a suite of educational and research experiences to introduce undergraduate students to the prospects and challenges of nanoscale science and engineering as part of a National Science Foundation Nanotechnology Undergraduate Education grant. Although open to all students, the program was designed in particular for engineering students whose curricula have relatively little flexibility. Activities were developed to fit into or to modestly supplement existing curricular frameworks, and were aimed at introducing students to three foundational aspects of nanoscale work: the underlying science, possible scientific and engineering applications, and the societal implications. A web site <http://nano.mtu.edu> was developed as central focal point for nano-related research and education activities at MTU.

The most successful activities included the creation of a new elective course on "Fundamentals of Nanoscale Science and Engineering"; a two-hour nanotechnology "exploration" for first-year engineering students and high school students; and summer research experiences for seven undergraduates. Beginning in the fall of 2005, a new interdisciplinary minor in "Nanoscale Science and Engineering (Nanotechnology)" became available to students. Major requirements for the minor include the above elective course, a new course in Societal Implications of Nanotechnology, a selection of approved elective courses outside of a student's major, and nanotechnology-related research or independent study.

This talk will outline these activities in more detail. Challenges, rewards, and lessons learned through the process of their development and implementation will also be presented.

A-13

Life in the nano world: the Molecularium project

Robert Vajtai, Shekhar Garde, Linda Schadler and Richard W. Siegel
Rensselaer Polytechnic Institute
Troy, NY 12180, USA

Similarly to the way a traditional planetarium experience takes us among planets and stars the Molecularium shows the way into the atomic and molecular universe; the building blocks of almost everything around and inside of us. The first, 20-minute show, developed originally for children in grades K-3 and designed for a planetarium setting, follows Oxy, Hydro, Hydra and Carbón—a cast of characters based on atoms—as they explore this inner universe. Their atomic-scale views are based on real molecular dynamics calculations and all of the involved positions and processes are scientifically authentic. The Molecularium project is part of the educational and outreach program of Rensselaer's NSF-funded Nanoscale Science and Engineering Center for Directed Assembly of Nanostructures. The web page of the project is <http://www.molecularium.com/>.

A-14**University Level Educational Issues Related to Nano-biotechnology : A Case Study**

Suranjan Panigrahi
North Dakota State University
Fargo, ND 58105 United States

Nano-biotechnology is an emerging and growing discipline that shows tremendous potential for solving various biological problems using different forms of nano-technology. Many universities have established courses/programs in nanotechnology areas. Many other universities are in the process of developing courses to train their future students in the broader context of nano- and nano- biotechnology. This presentation will summarize the acquired experience in developing a course on nano-biotechnology for the upper level undergraduate and junior level graduate engineering students at North Dakota State University (NDSU), Fargo. This course was originally developed at Cornell University's nano-biotechnology Center (NBTC) and has been made available to NDSU via distance education media for last three years. Overview on arrangements, inter-university collaborations, associated distance education and multimedia technologies will be presented. Cross-section of student's work as reflections of their learning and their acquired knowledge in nano-biotechnology will be illustrated. Moreover, the associated experience/challenges faced by the students in linking themselves with interdisciplinary subject matters (related to nano-biotechnology) will be reflected. The role of this collaborative arrangement in accelerating the opportunities to integrate nano-biotechnology for student's research/learning will also be reported. Finally, a general review and recommendation on developing university level course works related to nano-biotechnology using the available resources using inter-disciplinary and inter-university collaborations will be discussed.

A-15**Educating the Workforce for the New Nanotechnology Industry –
College of Nanoscale Science and Engineering at the University at Albany**

Pradeep Haldar, Robert Geer, Alain Kaloyeros
College of Nanoscale Science & Engineering,
University at Albany, SUNY
Albany, NY 12203 United States

The University at Albany's College of Nanoscale Science and Engineering (CNSE) – the first U.S. college in nanoscale science and technology – has evolved into an internationally recognized education and research center due to its eminently successful model for collaboration between industry, government and academia. The success of the NanoEngineering and NanoSciences graduate degree program relies on CNSE to continue to perform the critical function of providing an education to students of the highest quality equal or superior to that available in institutions of higher learning anywhere in the world. Moreover, CNSE is located in the most advanced research facilities of its kind at any university in the world. With a current net asset value in excess of U.S. \$2 billion, the 450,000-square-foot complex attracts over 150 corporate partners from around the world and offers faculty and students a one-of-a-kind academic experience in an interdisciplinary environment. CNSE's unique education and research experience is its integrated complex which currently houses over 1,000 faculty, researchers, and students from CNSE and its industrial partners, including IBM, Honeywell, GE, Infineon, SEMATECH, Applied Materials, and many others. As the college's new model matures and leadership advances, it continues to expand curricular offerings in Nanoeconomics, Nanobioscience and a dual Nano+MBA degree to participate in the development and implementation of CNSE's education, research, service, outreach and management programs to train the workforce of the nanotechnology industry.

B-1**Electron Transport in Molecular and Nano-scale Systems**

Shashi P. Karna

US Army Research Laboratory

Weapons and Materials Research Directorate

ATTN: AMSRD-ARL-WM

Aberdeen Proving Ground, MD 21005-5069

Electron transport in bulk materials forms the basis of the electronics technology and is well understood from the experimental and theoretical studies performed over the period of past five decades. Electron transport in quantum confined systems, such as molecules, quantum dots, and one-dimensional nanostructures, has recently attracted a great deal of attention due to the availability of new results made possible from the advancements in the experimental and theoretical techniques to create and explore nano-scale systems. This talk will explore the physics of electron transport in molecular and nano-scale systems and compare it with that in bulk materials.

B-2**Precisely Variational Quantum Chemistry via Analytical Density Functional Theory**

Brett Dunlap

US Naval Research Laboratory

Washington, DC 20375 United States

First-principles quantum chemistry is one of the most powerful tools to provide definitive information on the energy, forces between atoms, and their manifestations in molecules and solids. However, due to the very nature of quantum interactions between (two-body) and among (many-body) charged particles, the solution of the mathematical statements of the physics becomes dauntingly challenging--especially if meaningful numerical results are needed. Historical developments made by J. C. Slater and S. F. Boys in the 1950's, which introduce mathematically tractable functions for numerical calculations in quantum chemistry, lead directly to what we call analytic density-functional theory (ADFT). Its variational parameters are 10's of linear combination of atomic orbitals (LCAO) coefficients rather than 100's of plane-wave coefficients or numerical values at 1000's of points per atom per molecular orbital. In ADFT quantum-mechanical matrix elements are computed to machine precision. Only an analytic theory guarantees that one can always apply the variational principle to achieve whatever accuracy is necessary.

For small calculations ADFT scales as the number of orbitals cubed rather than the fourth power scaling of Hartree-Fock. The only major problem of ADFT is the labor-intensive optimization of our toolbox of analytic functional forms to achieve optimal results. In this talk, the toolbox of functionals developed by our group at US Naval Research Laboratory over the course of past 25 years will be described. We have used Perl scripts to optimize ADFT over the G2 and extended G2 sets of up to 148 molecules for various properties. The computer code is capable of rather accurate calculations of atomization energies, optimized geometries and dipole moments.

We use generalized Gaunt coefficients to speed up completely analytic, and thus precise, gradient calculations involving basis functions of high angular momentum. We have optimized the geometries of the most stable C240, C540, C960, C1500, and C2160 icosahedral fullerenes using a triple-zeta plus polarization orbital basis (6-311G*) and a matched basis for the Kohn-Sham potential that contains up to f functions. Even with a greatly simplified variational-quantum-chemical method calculations can still be challenging. Our largest calculation employing about 39000 basis functions could only be performed on a parallel-processing platform.

The Office of Naval Research, directly and through the Naval Research Laboratory, and the Department of Defense's High Performance Computing Modernization Program, through the Common High Performance Computing Software Support Initiative (CHSSI) Project MBD-5, supported this work.

B-3

Thermodynamics of Clusters : Size Sensitive Heat Capacities and Higher than Bulk Melting Point

Dilip Kanhere
Department of Physics
University of Pune
Pune, Maharashtra 411007 India

Recent experimental measurements on clusters in the size range of 20-200 have brought out a number of interesting features. Clusters of Tin and Gallium show melting point higher than bulk. The heat capacities of Gallium and Aluminium clusters show dramatic size sensitivity. We present results of ab initio molecular dynamics on a number of clusters. We establish a correlation between ground state geometry and the shape of heat capacity. Based on our extensive simulations we present our understanding of thermodynamics of finite size systems.

B-4

Stability of Nanoclusters and NDR Phenomena in Molecular Systems

Swapan Pati
J. N. Center for Advanced Scientific Research
Bangalore, Karnataka 560064 India

We have recently proposed some novel inorganic charge transfer (CT) complex like hetero-metallic Al-clusters. These Al-clusters have polarization responses 10000 times more than the conventional organic systems due to charge-transfer. We have also theoretically proposed the experimental strategies to synthesize these clusters. Transport through organic molecular species have attracted much attention due to their potential applications. We have recently proposed the mechanism behind negative difference resistance (NDR) in some of the Toul molecules. The talk will deal with the stability and transport mechanism of some of the nanomolecular systems.

B-5

Theory of Mössbauer Spectrum of a Single-Walled Carbon Nanotube

Vinod Tewary
Materials Reliability Division
National Institute of Standards & Technology
Boulder, Colorado 80305 United States

Identification of physical processes at the atomistic scale is necessary for characterization of nanomaterials, which is needed for their industrial application. Conventional methods of characterization of materials that depend upon their macroscopic response are not adequate for nanomaterials. We suggest that Mössbauer

spectroscopy can be a valuable new tool for quantitatively characterizing the nanomaterials at the atomistic scale because it depends directly upon their phonon spectra. In particular, we show that the Mössbauer spectra of single-walled carbon nanotubes (SWNTs) have some unusual features that can provide a new insight into the physical processes in SWNTs. We have calculated the line shapes of one phonon lines in the Mössbauer spectrum of ^{57}Fe in SWNTs of different chiralities and diameters using a phonon Green's function method which is also applicable to other nanomaterials. The phonons are represented in terms of causal Green's function that is calculated by using a Born-von Karman type model and the force constants derived from a recently constructed many body interatomic potential between carbon atoms in an SWNT. The effect of the Mössbauer isotope is represented by a change in the phonon Hamiltonian. The corresponding defect Green's function is calculated by solving the Dyson integral equation in the defect space. The phonon frequencies are calculated from the poles of the defect Green's function whereas the line shapes are obtained from its imaginary part. The line shapes can be measured and used to determine the chirality of SWNTs which can not be easily determined by any presently available method.

B-6

Surface Adsorption Effects on the Emission Properties of Single-Wall Carbon Nanotubes: A Density Functional Theory Study

Ruth Pachter
Materials & Manufacturing Directorate
USA Air Force Research Laboratory
Wright-Patterson Air Force Base, Ohio 45433-7702 United States

In order to explain field emission properties of single-wall carbon nanotubes (SWCNTs), we overview our theoretical work on the effects of surface adsorption, indicating that the results are consistent with experimental observations for O_2 , in preliminary work also for O_3 , and for Cs. Moreover, good agreement with experiment was obtained for changes in the Raman shifts upon alkali-atom adsorption in SWCNTs, and an understanding in terms of lattice expansion and charge transfer, further validating the calculations.

B-7

Multiscale Modeling with Carbon Nanotubes

Amitesh Maiti
Lawrence Livermore National Lab
Livermore, CA 94551 United States

Technologically important nanomaterials come in all shapes and sizes. They can range from small molecules to complex composites and mixtures. Depending upon the spatial dimensions of the system and properties under investigation, computer modeling of such materials can range from first-principles Quantum Mechanics, to Forcefield-based Molecular Mechanics, to Mesoscale simulation methods, to Finite-Element computation of properties. We illustrate all of the above modeling techniques through a number of recent applications with carbon nanotubes (CNTs): (1) effect of adsorbates on CNT-based field-emission displays [1]; (2) CNT-strain-controlled nano electromechanical sensor (NEMS) devices [2, 3]; (3) the sensitivity of topological defects on CNT action as chemical sensors [4]; (4) assessing the quality of metal-CNT contacts [5]; and (5) mesoscale morphology of polymer-CNT composites [6, 7] and finite-element computation of electrical and thermal transport [8].

- [1] A. Maiti, J. Andzelm, N. Tanpipat, and P. von Allmen, Phys. Rev. Lett. 87, 155502 (2001).
- [2] A. Maiti, A. Svizhenko, and M. P. Anantram, Phys. Rev. Lett. 88, 126805 (2002).
- [3] A. Maiti, News & Views, Nature Materials 2, 440 (2003).
- [4] J. Andzelm, N. Govind, and A. Maiti, Chem. Phys. Lett. 421, 58 (2006).

- [5] A. Maiti and A. Ricca, *Chem. Phys. Lett.* 395, 7 (2004).
- [6] A. Maiti, J. Wescott, and P. Kung, *Mol. Sim.* 31, 143 (2005).
- [7] A. Maiti, J. Wescott, and G. Goldbeck-Wood, *Int. J. Nanotechnology* 2, 198 (2005).
- [8] J. Wescott, P. Kung, and A. Maiti, to be published (2006).

B-8 **Theoretical Study on Exciton Dynamics of Dendritic Systems**

Masayoshi Nakano
Osaka University
Toyonaka, Osaka 560-8531 Japan

Excitation energy transport is one of the essential processes in photosynthesis in green plants on earth and also finds an important application in photonics and biology. Although typical energy transport is observed in supramolecular antenna involved in green plants and their artificial polymeric mimics, most of them have disordered structures, in which energy transport is partially carried out by random walk, thermal activation and so on. On the other hand, efficient and controllable energy transport is known to be one of the fascinating properties of dendritic systems with ordered fractal-like architecture, which exhibits a directed, multistep energy transport of absorbed light. The mechanism of this energy transport, which originates in exciton migration, in dendritic aggregate systems is investigated using a quantum master equation approach including exciton-phonon coupling. It is found that the overlap of exciton distributions between adjacent generations is essential for the efficient exciton migration in addition to the multistep exciton states originating from the fractal architecture. We also extend this approach to the calculation of exciton dynamics of supermolecular systems, i.e., dendrimers, based on the ab initio molecular orbital (MO) configuration interaction (CI) method. We examine the effects of the variation in the excitation energy of the core molecule of nanostar dendritic systems on the multistep exciton migration from the periphery to the core based on the relaxation factors among exciton states.

B-9 **Characterization of Nanostructures with Single Atom Sensitivity through Aberration-Corrected STEM**

Stephen Pennycook
Materials Science and Technology Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6030 United States

The aberration-corrected scanning transmission electron microscope (STEM) offers dramatically improved resolution and sensitivity for determining atomic arrangements, impurity concentrations and local electronic structure in nanostructured materials. Z-contrast images now reveal oxygen columns in perovskites, and individual atoms can be imaged and spectroscopically identified through electron energy loss spectroscopy. Coupled with density-functional calculations, the microscopic origins of many nanoscale properties are becoming understood. The location of charge carriers within the unit cell of the high temperature superconductor YBCO can be seen directly, the transfer of charge across a superconductor/ferromagnet interface relates to macroscopic properties, and spectroscopic imaging of charge ordering in manganese perovskites explains the nature of the phenomenon. The 3D shape and crystal polarity of high quantum yield semiconductor nanocrystals reveals their growth mechanism. Individual catalyst clusters can be imaged with single atom sensitivity, and theory reveals the room

temperature catalytic activity of gold nanocatalysts originates from low-coordination sites. Individual Hf atoms can be located in 3D within a Si/SiO₂/HfO₂ gate dielectric structure to a precision of 0.1 x 0.1 x 1 nm, and the perturbed electronic structure can be linked to macroscopic device properties.

B-10

Characterization of MW-CNTs synthesized by thermal and PE CVD for Display Devices

P. Ghosal, R. Sarkar, K. Muraleedharan, P. Chaturvedi*,

DS Rawal* and Harsh*

Defence Metallurgical Research Laboratory, Hyderabad 500058

*Solid State Physics Laboratory, Delhi 110054

Carbon nanotubes (CNTs) are a novel material system whose unique properties offer intriguing possibilities for the fabrication of nano-metric-scale molecular electronic devices. As a preliminary step towards realizing nanotubes, we have synthesized multiwall nanotubes in different conditions on silicon substrate using catalytic decomposition of acetylene. Carbon nanotubes has various applications in electronic field, such as display, IR detector array, cold cathode device etc. which require selective and patterned growth of carbon nanotubes.

Selectively grown vertically aligned CNTs provides much higher geometrical field enhancement leading to high emission current densities at low threshold field (for cold cathode device). Though plasma enhanced CVD (PECVD) generally enables more vertically aligned structure as compare to thermal CVD, we have deposited in both the methods to compare the structural details of the CNTs. In the process we have used patterned 20 nm dots made of iron, as catalyst for growth. These MWNTs are characterized using SEM, TEM and HRTEM. Among the various CNTs two different types of nanotubes are observed, closed internal caps bamboo structured multiwall nanotubes and hollow columnar uniform multiwall nanotubes. Along with the multiwall tubes of diameter ranging from 15 nm to 100 nm, we observed tubes with particles trapped inside and on tip of the tubes, which were analyzed using EELS/EDAX. TEM observation of these MWNT indicates that they are extremely resilient, capable of high levels of bending and tortional stress prior to fracture. Among the various parameters of growth/synthesis we have characterized their thickness, homogeneity, chemistry, spacing and bending and results are presented. Optimized conditions were used to obtain selective growth of carbon nanotubes on the patterned substrate and further produced the display devices.

B-11

Characterization of Nanoporous Diatom Frustules using Nanoindentation

Ghatu Subhash

Michigan Technological University

Houghton, MI 49931 United States

Diatoms are single-celled algae that inhabit both marine and fresh water environments. They form unique cell walls called frustules made of amorphous silica and are of size 20-100 microns. The frustules contain numerous nanosized pores arranged in a symmetric fashion. The frustules have been identified as potential sources for nanotechnological applications in filtration media, dies for nanotubes and nanofibers, and lithographic masks for manufacturing nano/micro scale features. Recent experimental studies using nano indenter have shown that the elastic modulus and hardness of the frustules are similar to those of silica, but their properties vary considerably with location. It has also been observed that the mechanical strength is inversely related to the size of frustules. The evolved failure patterns during nanoindentation were also

unique and complex. To gain further insight into these issues, a computational framework was developed where the indentation process has been simulated by a rigid-deformable contact process. A fixed orthogonal smeared crack model has been developed to simulate the initiation and propagation of fracture in the shell. Observed differences in the mechanical properties of the frustule due to the variation of indentation location and the influence of size and distribution of pores on the overall mechanical properties and failure patterns will be presented in detail.

B-12 **Nanolithography : Innovative Materials and Techniques**

Omkaram Nalamasu
Rensselaer Polytechnic Institute
Troy, NY 12180, USA

Lithography has been a fundamental driver of the miniaturization of circuits and associated productivity enhancements that form the basis for Moore's law. The advances in materials technology have propelled optical lithography to provide patterning solutions into sub-100 nm regime, well beyond the projected resolution limit of 2 μ m. In this presentation, I will detail the evolutionary and revolutionary material advances that have made the optical lithography the choice of technology for nanoelectronic device fabrication and illustrate how different nanolithography techniques can be utilized to fabricate structures for addressing a variety of technologically interesting problems.

B-13 **Nanoscience and the Energy Challenge: The U. S. Department of Energy's Nanoscale Science Research Centers**

Laura H. Lewis
Center for Functional Nanomaterials
Brookhaven National Laboratory
Upton, New York, United States

To support the synthesis, processing, fabrication and analysis at the nanoscale, the U. S. Department of Energy, Office of Science is developing, constructing and operating five new Nanoscale Science Research Centers (NSRCs). When complete, this network of five NSRCs will constitute the United States' premier User Facilities for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools and new computing capabilities.

The Brookhaven National Laboratory Center for Functional Nanomaterials (CFN), slated for initial operations in April 2007, will contain clean rooms, nanofabrication laboratories and one-of-a-kind signature instruments such as advanced electron microscopes. In addition to offering advanced equipment to the scientific community free of charge, the CFN also provides scientific expertise for basic research in support of energy: energy conversion, energy storage and energy efficiency. CFN research is concentrated in the fields of Nanocatalysis, Biological and Soft Nanomaterials and Electronic Nanomaterials. Recent research results selected from the three CFN scientific theme areas will be highlighted.

Acknowledgement: This research was supported in part by the U.S. Dept. of Energy, Division of Materials Science, Office of Basic Energy Sciences under contract DE-AC02-98CH10886.

B-14

Energy-Related Applications of Carbon Nanotubes Synthesized Using Novel Alloy Hydride Catalysts by Chemical Vapor Deposition Technique

Ramaprabhu Sundara
Department of Physics
Indian Institute of Technology Madras
Chennai, Tamil Nadu 600036 India

The talk presents the synthesis of different types of carbon nanotubes by the pyrolysis of suitable hydrocarbons over selective novel alloy hydride catalysts by the chemical vapour deposition (CVD) technique. The advantages of this novel approach to catalyst preparation using hydrogen decrepitation with reference to the increase in the catalytic reactivity and active sites for the formation of different types of CNTs are highlighted. The results of the characterization of the as-grown and purified CNTs by XRD, BET surface area analysis, SEM, TEM, HRTEM, TGA and Raman spectroscopy are described. The dependence of the yield and the purity of the CNTs synthesized on the alloy hydride catalysts are discussed. The energy-related applications of CNTs such as the oxygen reduction catalyst support material for proton exchange membrane fuel cell (PEMFC) and hydrogen storage capacity are discussed. The experimental techniques needed for these applications are described. The results of the performance studies of PEMFC and the hydrogen adsorption capacity of the purified MWNTs are discussed along with the recent literature reports.

B-15

Applications of Hybrid nanomaterials for Electrochemical Energy Storage

K. Vijayamohanan,
Physical and Materials Chemistry Division,
National Chemical Laboratory, Pune 411008, India.

Nano-structured hybrid materials have attracted much attention recently due to the possibility of tailoring their dimensionality to facilitate a change in their fundamental properties including redox potential, conductivity and charge storage in comparison with similar behavior of their bulk analogues. For example, the electron-transfer behavior of monolayer protected gold and silver nanoclusters have been found to vary dramatically with size. Similarly, the insertion of conducting polymers in layered host materials and other structurally organized environments can result organic-inorganic nanostructures with novel electrical, structural, and mechanical properties. Such systems can potentially show hybrid properties synergistically derived from both the host and the guest which could be profitably utilized for energy storage applications.

In the past, several layered, transition metal oxides and dichalcogenides have been used to prepare excellent lithium battery electrodes after intercalating Li^+ ions into them. Nevertheless, repulsive interactions between intercalated Li^+ cations put a strong limit on the efficiency. We here show that this problem could be solved by using a hybrid material (quasi two-dimensional lamellar nanocomposites) synthesized by chemically delaminating a layered host into molecular single layers like self-assembled monolayers. As a part of our continuing quest for preparing hybrid materials with novel or enhanced properties, we will discuss the application of these novel organo-inorganic structures as electrodes for rechargeable lithium batteries, supercapacitors and fuel cells.

References:

1. A novel approach to prepare poly(3,4-ethylenedioxythiophene) Nano-ribbons between V_2O_5 layers by microwave radiation, A. Vadivel Murugan et al **J. Phys. Chem.** 108(2004)10736

2. Self-assembled molecular nano-cathodes for rechargeable energy storage Modules, Trupti Maddanimath **Chemical Physics Letters**, 396(2004) 277-281.
3. Enhancement of double-layer capacitance behavior and its electrical conductivity in layered poly (3, 4 - ethylenedioxy thiophene) - based nanocomposite, A.V. Murugan, A. Kasi Viswanathan, Guy Campet, C.S. Gopinath, and K. Vijayamohanan **Appl. Phys. Let.**(2006) press

B-16

Novel Effect of Electron Irradiation in Nanostructures

Mauricio Terrones
IPICYT
San Luis Potosi, SLP 78216 Mexico

It will be demonstrated, that irradiation exposure at elevated temperatures, can be used as an effective tool to covalently weld SWNTs in order to create molecular junctions of various geometries. We have fabricated "Y", "X" and "T-like" junctions that are stable. Tight binding molecular dynamics calculations demonstrate that vacancies, formed under the electron beam, trigger the formation of molecular junctions involving seven or eight membered carbon rings. We envisage that our results will pave the way towards controlled fabrication of novel nanotube based molecular circuits, nanotube fabrics and network architectures. In this context, novel super architectures, using carbon as building blocks will be proposed and their mechanical and electronic properties discussed, as well as their possible applications.

We will also show that the melting and solidification behavior of metal crystals can be drastically altered when they are encapsulated in fullerene-like graphitic shells. The melting temperature of low melting point metal crystals (e.g. Bi, Sn, Pb, etc.) inside graphitic shells is increased relative to the bulk melting point by a much larger amount than that observed for metal crystals embedded in other materials. It appears that graphite is the ultimate material for enhancing the melting/solidification hysteresis of small crystals or clusters. Therefore, metal clusters encapsulated by graphitic shells may be potentially advantageous in temperature-resistant crystalline composite materials.

Finally, we demonstrate that controlled irradiation of multiwalled carbon nanotubes can cause large pressure buildup within the nanotube cores, to the extent of being able to plastically deform, extrude, and break solid materials that are encapsulated inside. We further show by atomistic simulations that the internal pressure inside nanotubes can reach values higher than 40 GPa. Nanotubes can thus be used as robust nanoscale jigs for extruding hard nanomaterials and modifying their properties, as well as templates for other high-pressure applications at the nanoscale.

C-1

Nanotechnology Research in India

Vikram Kumar
National Physical Laboratory
Delhi, India

C-2

Synthesis and study of characteristics of Nanomaterials for different applications

K. U. Bhasker Rao

Defence Materials Stores Research and Development Establishment,
G.T. Road, Kanpur 208 013

The science and technology of creating devices on nano scale and the renewed interest of material scientists to exploit the advantages of the Nano materials led to rigorous attempts by chemists for their synthesis. The potential applications of these nano devices in varied fields like medicine, communications, fuel cells, detectors & sensors, nano electrics etc. require a variety of materials in nano form. In addition to well known materials like fullerene, Carbon Nano tubes, methods have also been developed for obtaining metals and compounds in nano form to exploit their special properties for different applications. The status of synthesis in our laboratory of some of these materials and potential applications of these materials will be presented and discussed.

C-3

New Insights of Inorganic Nanotubes

Yoshio Bando

National Institute for Materials Science
Tsukuba, Ibaraki 305-0044 Japan

Synthesis and analysis of inorganic nanotubes, not necessarily containing graphitic carbon, have become an intriguing research topic over the last several years. Nowadays, inorganic nanotubes with interesting properties and potential applications constitute an important domain of the nanostructural family. Among these material systems, the nanotubes made of boron nitride, Si, III-N compounds, II-VI compounds, metal oxides are particularly important because of their unique properties and potential technological applications compared with conventional carbon nanotubes. It is of great interest to explore new synthesis pathways to form nanotubes of these materials; however, the reported tubular structures are either amorphous or polycrystal forms, which would negatively affect their performance in real application. So, the synthesis of single-crystalline nanotubes from these materials and exploration of their properties are challenging tasks yet to be accomplished.

We report herewith on a wide variety of novel inorganic nanotubes (covering the above inorganic materials) most recently synthesized and thoroughly analyzed within our Laboratory. New properties of these inorganic nanotubes, including optical, electrical, thermal, mechanical, and gas adsorbing will be demonstrated. In particular, the effective functions of these nanotubes filled by other foreign materials, such as liquid metal will be highlighted. The authors will take an advantage of the state-of-the-art high-resolution transmission electron microscopy for the microstructure analysis and novel properties associated with these inorganic nanotubes.

C-4

Shape matters in nanomaterials

Murali Sastry

Tata Chemicals Innovation Centre

Andheri (E), Mumbai 400 059, INDIA.

Development of synthetic protocols for controlling the shape of nanomaterials is one of the challenges facing researchers in nanoscience today. It is now recognized that in addition to size, the shape of nanoparticles influences their optoelectronic and catalytic properties. In this talk, I will briefly describe the research efforts in my group at growing anisotropic nanostructures by biological methods and at liquid-liquid and air-water interfaces. We have developed a method based on the UV-switchable reducing capability of Keggin ions to grow phase-pure metallic core-shell nanostructures and this will also be described. Aqueous gold ions may be phase transferred into non-polar organic solvents using a range of complexing ligands. I will conclude my talk with our experiments on using such phase-transferred gold ions in transmetallation reactions with organically dispersible silver nanoparticles leading to hollow and highly porous gold nanoparticles in a single step with excellent application potential in bio-imaging.

C-5

Novel Aspects of Property Control in Nanostructured Materials

Horst Hahn

Forschungszentrum Karlsruhe, Institute for Nanotechnology

Baden-Wuerttemberg 76344 Germany

Materials science is based on the understanding of the role of defects on the properties of materials. Popular examples are point defects for diffusion processes, dislocations for the plastic behavior of metals and alloys and interfaces playing an important role in phase transformation and electronic properties. The basic idea of nanostructured materials about 25 years ago was the incorporation of localized planar defects (grain or phase boundaries) with a large volume fraction, corresponding to grain sizes in the nanometer range, that novel properties arise based on the different atomic arrangements in the interfaces or due to the strong grain size dependence of the materials properties. A different approach is the use of homogeneously disordered materials, such as metallic glasses. Over decades, materials science has concentrated on the detailed understanding of the role of defects and processes to incorporate such defects even in larger concentrations to tailor the properties of such materials.

In semiconductors, the influence of electronic effects at interfaces between dissimilar materials has been extensively used to obtain properties necessary for advanced electronic devices. The properties of semiconductors can be altered reproducibly by applying external electric fields. Such tunable properties based on external fields have not been observed in metals and alloys, as the charges at surfaces or internal interfaces are screened and thus, do not alter the properties of a bulk materials. Recently, it has been shown in nanoporous metals and in thin films that the mechanical and electrical properties can be tuned when the metal is exposed to an electrolyte by the application of an electric field. The space charge regions at the interface between the electrolyte and the metal surface result in a re-distribution of electrons at the metal surface, i.e. a change in the Fermi energy. This effect is responsible for the tunability of the properties. As an example, substantial changes of the electrical conductivity have been observed in a nanoporous Au-Fe alloy and in a thin Au-film on a substrate at small potentials of a few Volt.

Furthermore, a novel technique for the preparation of unstable solid alloys of metals and ionic crystals is presented. It involves the deposition of neutral atoms or molecules as well as the deposition of ions controlled by an electric field. In the presentation the well established concepts of materials science are presented and are put in contrast with the new opportunities possible by using man-made nanostructures.

C-6**Carbon Nanotube Electrochemical (Bio)Sensors**

Ashwini K. Srivastava

Department of Chemistry, University of Mumbai

Vidyanagari, Santacruz (East), Mumbai – 400098, India

Electrochemical sensors are a class of devices that have found widespread use, ranging from the detection of gas molecules to the tracking of chemical signals in biological cells. Carbon materials have been used as components in electrochemical sensors for over a decade. Carbon nanotubes (CNTs) are promising materials for sensing applications due to their remarkable electrical, chemical, mechanical and structural properties. CNT can display metallic and semiconducting electron transport, possess a hollow core suitable for storing guest molecules and have largest elastic modulus of any known material. The chemical modification and solubilization of CNT represent an emerging area in the research on nanotubes based materials. The solubility of functionalized CNT in common organic solvent and/ or water offers unique opportunities toward developing CNT-based materials for chemical and biochemical modifications. This talk will focus on the application of functionalized CNTs for the development of nano-scale electrochemical (bio)sensors in the form of Chemically Modified Electrodes (CME) and Ion Selective Electrodes (ISE) for sensing and analyzing trace-levels of metals and biologically active materials, such as vitamins, amino acids, proteins, etc. The functionalized CNT based composite materials are characterized by spectroscopic and electrochemical methods and their potential windows are established. The cyclic and differential pulse voltammetric techniques are applied to study the interaction of functionalized carbon nanotubes with the targeted ions and molecules in dipolar aprotic solvent media. The results so obtained are utilized to develop carbon nanotubes based CME and ISE to target the analyte and miniaturize the sensor. An overview of the various design architectures used in fabrication of CNT based sensors and their utility will be presented in this talk.

C-7**Integrating and Accurate Positioning of 1D Nanowires in Devices and Circuits: Recent Developments, Current Challenges and Future Opportunities**

M. Saif Islam

University of California – Davis

Davis, CA 95616 United States

In the past few years, exciting developments in the synthesis and novel device demonstrations of one-dimensional (1D) semiconductor nanowires have given rise to an enormous optimism. Interesting characteristics such as high surface to volume ratio, quantum confinement, and simple and low cost synthesis process of nanowires are opening new frontiers in novel electronic and photonic devices. Despite a significant progress in nanowire synthesis and many promising single device demonstrations, nanowire applications have been stalled by our incapability to incorporate and precisely position them within devices and ICs. Several researchers have demonstrated a scheme of serially connecting metal electrodes to individual nanowires using slow and expensive e-beam lithography and explored numerous intriguing device opportunities. However, many of those methods are not likely candidates for cost-effective and mass-manufacturable integration process for reproducible fabrication of ultra-high density nanodevice arrays. This talk will give an overview of the recent developments, current challenges and future opportunities in the construction of large and complex systems with nanowires. We will present our novel nano-bridging techniques that can simultaneously connect a large number of highly directional metal-catalyzed nanowires between two pre-fabricated electrodes. The technique, for the first time, can help access individual nanowire based devices without using nano-probes or expensive lithography techniques. This method of connecting nanowires offers exciting opportunities of integrating III-V materials on Si

wafer for ultra-fast nano-electronic and photonic devices. A novel technique for positioning large arrays of free-standing nanowires with uniform size and spacing will also be presented for the first time.

C-8 **Electronics with Dyes**

Asim Kumar Ray
Queen Mary, University of London
London E1 4NS United Kingdom

Phthalocyanine (Pc) is a symmetrical 18 p-electron aromatic macrocyclic compound, having an alternating nitrogen atom-carbon atom ring structure closely related to the naturally occurring porphyrins. The Pc molecule is able to coordinate hydrogen and metal cations in its center by coordinate bonds with the four isoindole nitrogen atoms. Therefore, a variety of phthalocyanine complexes exist. A major application of phthalocyanine pigments is in the production of cyan printing inks used for printing paper and packaging materials. Nowadays, both metal-containing pigments and metal-free phthalocyanine pigments are commercially available and compete with one another. Apart from their high thermal and photostability they show intense absorption in the UV and red/near-ir regions of the spectrum. More recently, it is noted that phthalocyanines themselves have a remarkable range of semiconducting, photoconducting, optoelectronic, and non-linear optical properties in their own right. In Grätzel's photovoltaic cells, a dye is anchored to a TiO_2 surface; incoming light photoexcites the dye and an electron is injected in the conduction band of the substrate and the dye can be certain phthalocyanine derivatives. Films of several phthalocyanine derivatives have been extensively studied as sensitive elements of gas sensors. We have also fabricated single layer memory devices based on spun cast film of lead phthalocyanine molecules. A unique type of formulation in which lead sulphide nanoparticles are integrated into a thin film of phthalocyanine has recently been achieved to form inorganic/organic nanocomposites.

C-9 **Devices and Architectures for THz-Frequency Spectral Sensing at the Nanoscale**

Dwight Woolard
U.S. Army Research Office
U.S. Army Research Laboratory – ARO
RTP, NC 27709 United States

The U.S. Army Research Office (ARO) has strategic interests in advancing the state-of-the-art in nanoelectronic engineering towards new research applications that have relevance to national defense and security. Terahertz (THz) frequency spectral sensing has been one of these focus application areas for many years and one that is actively supported by the U.S. ARO, U.S. Army Edgewood Chemical Biological Center (ECBC) and U.S. Defense Threat Reduction Agency (DTRA) for its potential application towards the detection, identification and characterization of biological (bio) agents. Specifically, spectroscopic measurements conducted on biological materials and agents have produced spectral features within the THz frequency regime (i.e., ~ 300 GHz to 1000 GHz) that appear to be representative of the internal structure and characteristics of the biological samples that have been considered – e.g., DNA, RNA and bacterial spores. However, the THz spectroscopic approach is problematic in that the spectral features observed from bulk samples of the biological materials tends to be very weak (i.e., ~ 1-5% local variation in spectral absorption) and of limited number within the band (i.e., < 50-100 spectral features). One fundamental approach for avoiding the previously cited limitations is to prescribe novel techniques whereby the THz-frequency absorption signatures could be collected from individual biological molecules at the nanoscale. To this end, ARO, ECBC and DTRA have launched numerous research efforts that seek to develop new devices and architectures that will be effective in extracting THz signatures from target bio-molecules. This

presentation will overview a number of multidisciplinary research projects focused the engineering demonstration of novel devices and architectures that have promise for THz-frequency sensing and imaging at the nanoscale.

C-10 **Protein Nanosensors for Multi-Scale Technologies**

Craig Friedrich
Michigan Technological University
Houghton, MI 49931 United States

The Multi-scale Technologies Institute at Michigan Technological University is focused on integrating technologies with characteristic dimensions that span many orders of magnitude. This presents many exciting opportunities and challenges requiring an interdisciplinary approach. One of these applications is a nanosensing platform that utilizes quantum dots, proteins, and single electron transistors (SETs) to form a chemical or biological detection system.

Quantum dots (QDs) are nanometer scale crystals of semiconductor materials. When excited by light of a wavelength shorter than their emission wavelength, the dots emit at a Stokes-shifted characteristic emission wavelength. By functionalizing the exterior of the QDs with environmentally sensitive molecules, such as amino acids, the emission characteristics of the QDs will change. This change can be optically detected. Bacteriorhodopsin (bR) is an optical protein extracted from the cell membrane of an extremophile bacterium. bR converts light to electrical charge very efficiently and with no cross-talk among adjacent molecules. bR serves as the optical-to-electrical transduction medium in the nanosensor system. To reduce the size and power of the sensing system, SETs will be used to sense the bR output. The bR, when coupled with the SETs, will form an array of nano-optical field effect transistors giving a small and very low power nanosensor system. The talk will focus on the system aspects of the application and report on progress to date.

C-11 **Imaging Spermatozoa using Atomic Force Microscopy – A Valuable Tool for Research in Contraceptive Development**

Koel Chaudhury
School of Medical Science and Technology
Indian Institute of Technology, Kharagpur
Kharagpur, West Bengal 721302 India

The ability to image living biological cells in three dimensions in their native environment at atomic resolution has made atomic force microscopy (AFM) a valuable tool for research in biology and related areas. One of the interesting applications of AFM is in the field of reproductive biology. Unstained, unfixed spermatozoa in their natural physiological surroundings provide extensive information on the morphological and pathological defects in sperm cells with precise topographical details. Sperm head defects and the acrosome at the tip of the head, responsible for fertilization, can be examined and correlated with the lack of functional integrity of the cell. Considerable amount of work has been done on sperm chromatin analysis using AFM. Rigorous research by our group over the past two decades has led to the development of a non-hormonal, reversible male contraceptive given the name RISUG® (an acronym for Reversible Inhibition of Sperm Under Guidance). Non-contact mode AFM was used to examine the morphological and topographical alterations on the sperm surface induced by this contraceptive, *in vitro*. An almost complete disintegration of the plasma membrane with subsequent rupture of the acrosomal membrane leading to dispersion of acrosomal contents was observed. Clustering of the mitochondria in the midpiece region and its fusion with sperm head indicated loss of functional competence of the

spermatozoa. AFM, with its ability to provide morphological details and 3D topographical images of the spermatozoa at nano-resolution, appears to have a tremendous potential as an investigative research tool in facilitating contraceptive development and/or improving infertility management.

C-12

Implication of nanotechnology and future health effects: Biological interaction of engineered nanomaterials

Saber Hussain, Andrew Wagner, Amanda Schrand, Cat Carlson, Christin Grabinski, and John Schlager

Applied Biotechnology Branch,
Air Force Research Laboratory,
Wright-Patterson AFB, OH 45434

Nanotechnology involves the creation and manipulation of materials at the nanoscale level to produce unique products with novel properties. Nanomaterials, which are defined functionally as have a single dimensional feature within the 1 - 100 nanometers range, have been used to create materials that exhibit novel physicochemical properties and function imparted through this engineered, controlled feature size. Although nanomaterials are currently being widely used in advancing technology, there is a serious lack of information concerning the human health and environmental implications of manufactured nanomaterials. The assessment of nanoparticle potential adverse impact should be a fundamental requirement before large-scale production and technological implementation of novel materials. In view of their possible effect on human health our main focus is to define and/or classify nanoparticles based on the nature of their toxicity. The main focus of this presentation will be to discuss basic research applied to discover biological interaction of nanomaterials and its relationship to potential human health concerns. The results will be presented on interaction of nanomaterials, size dependent toxicity and potential mechanism of toxicity in various in vitro cell models. The use of these quick assessment in vitro reference studies on toxicity, serve to uncover critical mechanisms of toxic effects associated with nanoparticle interaction with the biological molecules.

C-13

Applications of Nanoscale Sciences to Cell Wall Biotechnology in Trees

Chandrashekhar P. Joshi,
School of Forest Resources and Environmental Sciences,
Michigan Technological University,
Houghton, MI 49931, United States

Forest product industries produce thousands of wood products from trees that are vital for sustaining global economies and exploding human populations. Trees also mitigate the evil effects of increased green house gases by sequestering excess amounts of atmospheric carbon into wood for a long time. Thus biotechnological improvements in wood formation hold a tremendous promise from economical as well as ecological perspectives. Biologically, wood is nothing else but cell walls of dead xylem cells those help conducting water and minerals to the top of the tree and provide mechanical strength to tree trunks so that trees can withstand environmental assaults for hundreds or even thousands of years. For over 300 million years, trees have been producing cellulose Nanofibrils that further interweave with themselves as well as other cell wall polymers such as hemicelluloses and lignin to produce Nanocomposites that we call wood. Our main goal is to first understand the molecular processes by which trees accomplish this feat and then genetically engineer wood formation to improve the end-products for human utilization. Towards this goal, we have dissected the contribution of several genes to wood formation and produced novel wood phenotypes. Little is known about the biological processes that dictate a variety of wood quality traits and

ultra-sensitive Nanotechniques are required to catalogue the existing natural variations in wood traits. Finally, changes in wood gene expression at the single cell level must be monitored. Advancements in Nanotechnology could thus be harnessed for studying the process of wood formation at the Nanoscale level, for detection of physical changes in wood resulting from genomic modifications or natural variations, and for monitoring Nanochanges in gene expression levels by using whole genome-wide Nanoarrays based on carbon Nanotubes. Availability of such Nanochips will also open up new avenues in medicine, homeland security, and biology. Manipulation of the cell wall nanostructures of trees will allow us to create novel wood products that would possess superior qualities for end-utilization. An active cross-disciplinary cooperation among scientists and engineers is indispensable for attainment of this goal.

C-14

Biobased Organic Synthesis: Novel Building Blocks for Soft Nano Materials by Bottom-Up Design

George John
The City College of New York, CUNY
New York, NY 10031 United States

The self-assembly of low molecular weight building blocks into nanoscale molecular objects has recently attracted considerable interest in terms of the bottom-up fabrication of nanomaterials. The building blocks currently used in supramolecular chemistry are synthesized mainly from petroleum-based starting materials. However, bio-based organic synthesis presents distinct advantages for the generation of new building blocks since they are obtainable from renewable resources. This study is an effort to combine the philosophies of green chemistry and supramolecular chemistry, making use of renewable plant-derived resources as the starting materials (an alternate feedstock) for the noncovalent synthesis of meso- and nanoscale structures. The use of cardanol and its derivatives for various applications is well known. However its use in the synthesis of aryl glycolipids and their self-assembled nanostructures are new to the literature. The glycolipids are self-assembled to form a variety of well-defined nanostructures including liquid crystalline phases (thermotropic & lyotropic), vesicles, nanofibers, low-molecular weight gelators and nanotubes under suitable conditions, which could be of use in material applications. We have developed multiple systems based on biobased organic synthesis by chemical/biocatalytic methods for functional applications. These results will lead to efficient molecular design of supramolecular nanostructures and nanomaterials based on green chemicals, otherwise under-utilised. Also address the advances that have led to the understanding of chiral behaviour and the subsequent ability to control the structure of glycolipid nanostructures-derived from renewable resources-and the resulting impact of this on future material applications.

C-15

Designing micro, macro, and nano artificial cells: potentials and limitations

S. Prakash
Department of Biomedical Engineering and Physiology
McGill University
Montreal, QC, H3A 2B4 Canada

Artificial cell microcapsules are known to have excellent application in engineering, medicine, biotechnology and others. The biggest challenge however is to design artificial cell capsules with specialized features useful for target specific applications. A novel approach in micro, macro and nano capsule design will be discussed. In addition recent development in artificial cell design for use in renal failure, colon cancer, CD, and IBD therapy procedures using micro, macro and nano capsule will be discussed.